

# **Burn (BUR) Package Reference Manual**

The Burn (BUR) package models the combustion of gases in control volumes. The models consider the effects of burning on a global basis without modeling the actual reaction kinetics or tracking the actual flame front propagation. The BUR package models are based on the deflagration models in the HECTR 1.5 code. New in MELCOR 1.8.5 is a diffusion flame model, also derived from HECTR 1.5.

This Reference Manual describes the models employed in the BUR package. Detailed descriptions of the user input requirements can be found in the BUR Package Users' Guide.

# BUR Package Reference Manual

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# BUR Package Reference Manual

## 1. Introduction

The Burn (BUR) package models the combustion of gases in control volumes. These models consider the effects of burning off premixed gases without modeling the actual reaction kinetics or tracking the actual flame front propagation. The models in the BUR package are based on the deflagration models in the HECTR 1.5 code [1]. The only significant modifications made were to provide more direct user control of the models through the implementation of sensitivity coefficients and to include optional model parameters that are used to override the nominal parameters in control volumes in which direct containment heating (DCH) is occurring.

A diffusion flame model is available in MELCOR 1.8.5, also based on HECTR 1.5. The diffusion flame model allows more realistic modeling of DCH phenomena without having to make major adjustments to the nominal bulk burn parameters.

Briefly, a burn is initiated if certain criteria are satisfied in a control volume, causing the reactants (hydrogen, carbon monoxide and oxygen) to be converted during the burn to steam and carbon dioxide. The conversion occurs over a time interval called the burn duration. The reaction may or may not be complete, depending on the conditions in the control volume. After a burn is initiated in a control volume, it can be propagated to adjoining control volumes if a second set of criteria is satisfied. These criteria, as well as the duration and completeness of the burns, are discussed in Section 2. The modeling follows the recommendations of the MELCOR Assessment on Combustible Gas Treatment [2]. The default values and correlations used to calculate burn effects are those used in Reference 1.

For user convenience, the BUR package also prints messages to warn the user when the detonability criteria are satisfied in a control volume. A *detonation* is combustion in which the flame front travels at supersonic speeds, whereas a *deflagration* travels at subsonic speeds. In the BUR package, only deflagrations are modeled; detonations are merely flagged and no other action is taken.

The gases hydrogen ( $H_2$ ), carbon monoxide (CO), carbon dioxide ( $CO_2$ ), and oxygen ( $O_2$ ) must be defined in the NonCondensable Gas (NCG) package whenever the BUR package is active. Steam ( $H_2O$ ) is automatically present for all MELCOR calculations, so no special action need be taken to include it in a calculation.

The BUR package currently has a limited capability to burn deuterium gas ( $D_2$ ). For purposes of combustion,  $D_2$  is treated as equivalent to  $H_2$  on a mole-for-mole basis. Therefore, one mole of  $D_2$  will combine with one-half mole of  $O_2$  to produce one mole of  $H_2O$  (not  $D_2O$ ), and mass will not be conserved. Some equivalence must be assumed in the absence of a  $D_2O$  equation of state comparable in quality to the equation of state used in MELCOR for  $H_2O$ . Equivalence on a molar basis was chosen because the equations of state of  $D_2O$  and  $H_2O$  are much more similar on a molar basis than on a mass basis,

particularly in the gas phase. In addition, the former gives a more accurate value for the heat of combustion.

The same mole-for-mole equivalence is assumed in ignition, detonation, and completeness calculations, and input (or default) data for  $H_2$  will be applied to  $D_2$  and  $H_2/D_2$  mixtures. We believe that the error is small: for example, the ideal combustion limits for  $D_2$  are 5.0 to 95.0 mole percent compared to 4.0 to 94.0 mole percent for  $H_2$ .

## 2. Detailed Models

In the following equations, variables that are defined by user input are referred to by the same names as described in the Burn Package Users' Guide. Thus, there is a direct correspondence between the variables in the Users' Guide and those in the Reference Manual.

### 2.1 Burn Model Logistics

A burn is initiated in a control volume if the ignition criteria discussed in Section 2.2 are satisfied. As soon as a burn is initiated, calculations (described in Sections 2.3 and 2.4) are performed to determine the completeness of the burn and its duration. During subsequent timesteps, the reactants are converted to the products of combustion in that control volume according to the reactions.



The rate of burning varies during the burn duration to account for change in composition, e.g., due to inter-compartment flow and gas sources, as described in Section 2.5.

After a burn is initiated in a control volume, it can be propagated to adjoining control volumes if a second set of criteria is satisfied. These criteria are discussed in Section 2.6. After a burn propagates into a control volume, the same steps as outlined above for ignition are followed to calculate the burn effects.

## 2.2 Ignition Criteria

A deflagration is initiated in a control volume if the mole fraction composition satisfies the criteria described in this section. In addition, control volumes that are specified to contain igniters are tested against different criteria than control volumes without igniters, and a separate criteria may be specified for use when direct containment heating (DCH) is occurring in a control volume. For all cases, LeChatelier's formula (for the effective combustion mole fraction for a mixture containing more than one combustible gas) is used to determine the threshold of ignition. In particular, ignition occurs when the following criteria is satisfied:

$$X_{H_2} + X_{CO} \left( \frac{L_{H_2,ign}}{L_{CO,ign}} \right) \geq L_{H_2,ign} \quad (2.3)$$

where

$X_{H_2}$  = hydrogen mole fraction in the control volume;

$X_{CO}$  = carbon monoxide mole fraction in the volume;

$L_{H_2,ign}$  = XH2IGN, if there are no igniters in the volume and DCH is not occurring,

or

XH2IGY, if there are igniters in the volume and DCH is not occurring,

or

XH2DCH, if DCH is occurring in the volume;

$L_{CO,ign}$  = XCOIGN, if there are no igniters in the volume and DCH is not occurring,

or

XCOIGY, if there are igniters in the volume and DCH is not occurring,

or

XCODCH, if DCH is occurring in the volume;

XH2IGN = hydrogen mole fraction limit for ignition without igniters, when DCH is not occurring, input on record BUR001 (default = 0.10);

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XH2IGY = hydrogen mole fraction limit for ignition with igniters, when DCH is not occurring, input on record BUR001 (default = 0.07);

XH2DCH = hydrogen mole fraction limit for ignition during DCH, input on record BUR001 (default = XH2IGY);

XCOIGN = carbon monoxide mole fraction limit for ignition without igniters, when DCH is not occurring, input on record BUR001 (default = 0.167);

XCOIGY = carbon monoxide mole fraction limit for ignition with igniters, when DCH is not occurring, input on record BUR001 (default = 0.129);

XCODCH = carbon monoxide mole fraction limit for ignition during DCH, input on record BUR001 (default = XCOIGY).

The preceding tests are made only for the presence of sufficient combustible gases. Tests are also made to determine whether there is sufficient oxygen and to determine whether the amount of steam and carbon dioxide is below the inerting level. The same values are used when igniters are present as when there are no igniters, but separate values may be specified for use during DCH. The ignition and inerting criteria are

$$X_{O_2} \geq XO2IG \text{ (or } XO2DCH \text{ during DCH)} \quad (2.4)$$

$$X_{H_2O} + X_{CO_2} < XMSCIG \text{ (or } XINDCH \text{ during DCH)} \quad (2.5)$$

where

$X_{O_2}$  = oxygen mole fraction in the control volume;

$X_{H_2O}$  = steam mole fraction in the control volume;

$X_{CO_2}$  = carbon dioxide mole fraction in the volume;

XO2IG = minimum oxygen mole fraction for ignition, input on record BUR001 (default = 0.05);

XO2DCH = minimum oxygen mole fraction for ignition during DCH, input on record BUR001 (default = XO2IG);

XMSCIG = maximum diluent mole fraction for ignition, input on record BUR001 (default = 0.55);

XINDCH = maximum diluent mole fraction for ignition during DCH, input on record BUR001 (default = XMSCIG).

If all three tests are satisfied (Equations (2.3) through (2.5)), i.e., there is enough hydrogen and/or carbon monoxide, enough oxygen, and not too much steam and/or carbon dioxide, a burn is initiated. The burn duration and combustion completeness are discussed in Sections 2.3 and 2.4. If too much steam and carbon dioxide is present, the control volume is considered to be inert, and is identified as such in the printed edits. A message is printed to the output file and to the special message file and a plot dump is written (if specified by the user) when a deflagration begins and ends in any control volume.

### 2.3 Combustion Completeness

In MELCOR, deflagrations are not required to be complete; that is, all of the combustible gases present in a control volume at the start of a deflagration are not required to be burned during the deflagration. The *combustion completeness* is used to determine the amounts of combustible gases that should be present in a control volume at the end of an incomplete burn. In the BUR package, the combustion completeness, CC, is defined as

$$CC = 1 - \frac{Y_{min}}{Y_{max}} \quad (2.6)$$

where Y is given by the LeChatelier formula,

$$Y = X_{H_2} + X_{CO}(YH_2CC/YCOCC) \quad (2.7)$$

and

$Y_{max}$  = value of LeChatelier formula evaluated at the start of the burn (initial amount of combustibles);

$Y_{min}$  = value of LeChatelier formula that is desired at the end of the burn (final amount of combustibles);

$YH_2CC$  =  $XH_2CC$ , if DCH is not occurring, or  
           =  $XH_2CCD$ , if DCH is occurring;

$YCOCC$  =  $XCOCC$ , if DCH is not occurring, or  
           =  $XCOCCD$ , if DCH is occurring;

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XH2CC = hydrogen mole fraction for calculating combustion completeness, input on record BUR003 (default = 0.08);

XH2CCD = hydrogen mole fraction for calculating combustion completeness during DCH, input on record BUR003 (default = XH2CC);

XCOCC = carbon monoxide mole fraction for calculating combustion completeness, input on record BUR003 (default = 0.148);

XCOCCD = carbon monoxide mole fraction for calculating combustion completeness during DCH, input on record BUR003 (default = XCOCC).

The combustion completeness is first evaluated by the method described below, then it is used to determine the value for  $Y_{min}$  for the current deflagration in the control volume. The burning rate is adjusted as necessary (see Section 2.5) to achieve this value at the end of the burn.

The combustion completeness can be input as a constant value, calculated from a user-specified control function, or calculated from a correlation. The default correlation for combustion completeness, which was obtained from the HECTR 1.5 code [1], and derived from experimental data, is dependent on the mole fraction of combustible gases present at the start of the burn,  $Y_{max}$ , and is given by

$$CC = 0.0 \text{ for } Y_{max} \leq 0.03746 \quad (2.8)$$

$$= 23.4116(Y_{max} - 0.03746) \text{ for } Y_{max} > 0.03746 \quad (2.9)$$

The constants in this correlation have been implemented in sensitivity coefficient array 2202.

### 2.4 Burn Duration

The burn duration is calculated by dividing a user-specified characteristic dimension by the *flame speed*. The flame speed can be input as a constant value, calculated from a user-specified control function, or calculated from a correlation. Optional input can be specified to determine the flame speed with a different constant, control function or correlation when DCH is occurring in the control volume. The default correlation, obtained from the HECTR 1.5 code, was derived from experimental data. However, few data were available regarding the effect of large amounts of diluents (steam and carbon dioxide) on flame speed, so the correlation is questionable in mixtures with high diluent concentration. For these mixtures, sensitivity studies should be conducted to bound the expected pressure rises. The default correlation for the flame speed,  $V$ , is

$$V = V_{base} \times C_{dil} \quad (2.10)$$

where

$$V_{base} = 59.2Y_{max} + 1.792 \text{ if } 0.0 \leq Y_{max} \leq 0.1, \quad (2.11)$$

$$= 172.88Y_{max} - 9.576 \text{ if } 0.1 < Y_{max} \leq 0.2, \quad (2.12)$$

$$= 50.Y_{max} + 15. \text{ if } 0.2 < Y_{max} \leq 0.3, \quad (2.13)$$

$$= -50.Y_{max} + 45. \text{ if } 0.3 < Y_{max} \leq 0.4, \quad (2.14)$$

$$= -75.Y_{max} + 55. \text{ if } 0.4 < Y_{max} \leq 0.6, \quad (2.15)$$

$$= -64.3Y_{max} + 48.58 \text{ if } 0.6 < Y_{max} \leq 1.0 \quad (2.16)$$

$$C_{dil} = \max(0.05, 1.0 - 4.53XD + 5.37XD^2) \text{ if } 0.0 \leq Y_{max} \leq 0.2 \quad (2.17)$$

$$= \max(0.05, 1.0 - 4.53XD) + 5.37XD^2(0.3 - Y_{max})/0.1 \\ + \max(0.0, 1.0 - 1.29XD)(Y_{max} - 0.2)/0.1 \text{ if } 0.2 < Y_{max} \leq 0.3 \quad (2.18)$$

$$= \max(0.0, 1.0 - 1.29XD) \text{ if } 0.3 \leq Y_{max} \leq 1.0 \quad (2.19)$$

$XD$  = diluent concentration ( $X_{H_2O} + X_{CO_2}$ ).

The constants in this correlation have been implemented in sensitivity coefficient array 2200. The burn duration time,  $t_{comb}$ , is calculated by dividing the flame speed into a user-specified characteristic dimension of the control volume, CDIM (or CDDH when DCH is occurring), input on record BUR1XX:

$$\begin{aligned} t_{comb} &= CDIM / V \text{ if DCH is not occurring or} \\ &= CDDH / V \text{ if DCH is occurring.} \end{aligned} \quad (2.20)$$

## 2.5 Combustion Rate

The combustion rate (amount of hydrogen, carbon monoxide, and oxygen converted to steam and carbon dioxide per timestep) is not constant during a burn. Rather, it is adjusted at each timestep to account for inter-compartment flows and gas sources in an effort to match the desired final conditions. In other words, the combustion rate is adjusted so that the mole fractions corresponding to the calculated combustion completeness and the desired burn duration are simultaneously achieved. At each timestep, the burn rate, YRATE, is calculated as

$$YRATE = (Y(t) - Y_{min}) / (t_o + t_{comb} - t) \quad (2.21)$$

where

$t_o$  = time that burn was initiated, and

$t$  = current time in calculation.

Once the rate is calculated, it is used to determine the decrease in the inventory of the combustible gases for the current MELCOR system timestep:

$$DELH2 = X_{H2}(t) \cdot YRATE \cdot \frac{DT}{Y(t)} \quad (2.22)$$

$$DELCO = X_{CO}(t) \cdot YRATE \cdot \frac{DT}{Y(t)} \quad (2.23)$$

where

$DELH2$  = decrease in hydrogen moles in the control volume during the timestep from combustion,

$DELCO$  = decrease in carbon monoxide moles in the control volume during the timestep from combustion, and

$DT$  = MELCOR system timestep (s).

At the end of the burn, the value  $Y_{\min}$  would be reached exactly if there were no flow or sources. These values are updated on every timestep to reflect the changing conditions. DELH2 and DELCO are constrained to prevent burning more moles of either gas than are present in the control volume.

The energies of formation are included in the water and noncondensable gas equations of state. With this formulation, simply changing the relative masses of the reactants and products will automatically result in the appropriate pressure and temperature increase. Thus, it is not necessary to calculate a combustion energy release to a control volume. The total mass and energy of a control volume are not changed by the BUR package, but the masses of individual species are changed to reflect the reactions listed in Section 2.1. (That is, DELH2, DELCO, and  $0.5 \cdot \text{DELH2} + 0.5 \cdot \text{DELCO}$  moles of hydrogen, carbon monoxide, and oxygen are subtracted from the control volume while DELH2 and DELCO moles of steam and carbon dioxide are added to the control volume.) Because the specific enthalpy of each species properly accounts for the energy of formation, the conversion of the reactants to the products increases the temperature and pressure of the control volume with combustion, even though the total energy remains unchanged.

## 2.6 Propagation Criteria

Propagation of combustion from a control volume to connected control volumes is allowed after a user-controlled time period has elapsed. This delay is intended to account for the time it would take for a flame to reach the edge of a control volume if a flame front were actually being modeled. Different delay periods may be specified depending upon whether or not DCH is occurring in the control volume. Propagation will then occur if the propagation criteria are satisfied in the connected control volume. The propagation delay,  $t_{\text{prop}}$ , is calculated to be

$$t_{\text{prop}} = \text{FRAC} \cdot t_{\text{comb}} \quad (2.24)$$

where

$\text{FRAC}$  = TFRAC, if DCH is not occurring in the control volume, or

= TFDH, if DCH is occurring in the control volume; and

$\text{TFRAC}$  = propagation time fraction input on record BUR1XX (default = 0)

$\text{TFDH}$  = override value of TFRAC during DCH, input on record BUR1XX (default = TFRAC).

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Note that if TFRAC equals zero, propagation is possible as soon as a control volume begins burning. If TFRAC equals 1.0, propagation is only considered at the end of the control volume burn.

For propagation, LeChatelier's formula is still applicable if appropriate values are used for the L parameters. Propagation is allowed if the following inequality is satisfied

$$X_{H_2} + X_{CO} (L_{H_2,prp} / L_{CO,prp}) \geq L_{H_2,prp}$$

where

$L_{H_2,prp}$  = XH2PUP, for upward propagation, or  
= XH2PHO, for horizontal propagation, or  
= XH2PDN, for downward propagation;

$L_{CO,prp}$  = XCOPUP, for upward propagation, or  
= XCOPHO, for horizontal propagation, or  
= XCOPDN, for downward propagation;

XH2PUP = hydrogen mole fraction limit for upward propagation, input on record BUR003 (default = 0.041).

XH2PHO = hydrogen mole fraction limit for horizontal propagation, input on record BUR003 (default = 0.06).

XH2PDN = hydrogen mole fraction limit for downward propagation, input on record BUR003 (default = 0.09).

XCOPUP = carbon monoxide mole fraction limit for upward propagation, input on record BUR003 (default = 0.125).

XCOPHO = carbon monoxide mole fraction limit for horizontal propagation, input on record BUR003 (default = 0.138).

XCOPDN = carbon monoxide mole fraction limit for downward propagation, input on record BUR003 (default = 0.15).

The propagation direction is determined directly from the flow path input using the *from* and *to* elevations (see the FL Package Users' Guide). If a flow path is not open, or if the flow path is covered by water, propagation is not allowed. Note that the presence of a check valve is not taken into account when determining whether a flow path is open.

A message is printed to the output file and to the special message file and a plot dump is written (if specified by the user) when a deflagration due to propagation begins in any control volume.

## 2.7 Detonation

MELCOR does not contain a detonation model. However, tests are performed in each control volume, and a warning message is written indicating the possibility of a detonation if all of the following mole fractions limits are satisfied:

$$X_{H_2} > XH2DET \quad (2.25)$$

$$X_{O_2} > XO2DET \quad (2.26)$$

$$X_{H_2O} < XH2ODT \quad (2.27)$$

where

XH2DET = minimum hydrogen mole fraction for detonable mixture, input on record BUR002 (default = 0.14),

XO2DET = minimum oxygen mole fraction for detonable mixture, input on record BUR002 (default = 0.09), and

XH2ODT = maximum steam mole fraction for detonable mixture, input on record BUR002 (default = 0.30).

No detonation calculation is performed when a detonable mixture is detected. The warning message is written, but the calculation continues under the control of the deflagration model. The detonation model is mainly intended as a user convenience to flag potentially dangerous conditions that may require separate analysis.

## 2.8 Diffusion Flame Model

The diffusion flame model is intended to model the burning of hydrogen entering a control volume under DCH conditions. Under such conditions, the hydrogen enters accompanied by hot melt particles which act as igniters, so that the conditions for ignition and burning are quite different from those for a bulk burn. The diffusion flame implementation is a simple model that burns combustible gas passing through a flow path and entering a control volume containing oxygen, subject to ignition criteria. These are defined on the

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BUR005 input records (see BUR Users Guide), new in MELCOR 1.8.5. This general approach is used both in MELCOR and in CONTAIN.

As implemented in MELCOR, a combustion completeness criterion is used as specified on the BURCFxx cards and described in the BUR Users Guide. No flame speed or duration calculation is performed, and the ignition criteria are the same as for deflagration. Additionally, the airborne DCH debris temperature must be greater than a lower limit specified by the C2203 sensitivity coefficient (default = 600K). See BUR Users Guide.

The ignition limits for the diffusion flame model are set to insure virtually complete combustion with any oxygen present in the receiving volume even if large amounts of inerting gases are present. This is done to simulate the expected effect of hot DCH debris in the incoming gas on hydrogen recombination, and is similar to the model used in calculating DCH with CONTAIN3. The diffusion flame implementation assumes burning occurs whenever the ignition criteria are met. The effects of flashback or blowout are not considered. (Note: flashback occurs when the flame is swallowed back into the combustible gas source; blowout occurs when the flame front moves away from the gas source so rapidly that it is extinguished).

### 3. Timestep Control

When a burn first occurs, the Burn Package requests a fallback after which the calculation continues with the timestep value specified by the BURTIM record. In addition, as the burn approaches completion, tests are included to prevent excessive overshoot of the originally-desired burn completeness values. In particular, a timestep is repeated if the originally-desired burn completeness values are crossed during that timestep and either (a) the combustible gas concentration is more than 0.5% different, or (b) the diluent concentration is more than 1% different from the originally-desired burn completeness values. These maximum overshoots can be adjusted through sensitivity coefficient C2201.

### 4. References

- 1 S. E. Dingman, et al., HECTR Version 1.5 User's Manual, SAND86-0101, NUREG/CR-4507 (April 1986).
- 2 G. G. Weigand, ed., Thermal-Hydraulic Process Modeling in Risk Analysis: An Assessment of the Relevant Systems, Structures, and Phenomena, SAND84-1219, NUREG/CR-3986 (August 1984).
- 3 K. K. Murata et al., Code Manual for CONTAIN 2.0: A Computer Code for Nuclear Reactor Containment Analysis, SAND97-1735, NUREG/CR-6533 (December 1997).